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Contents

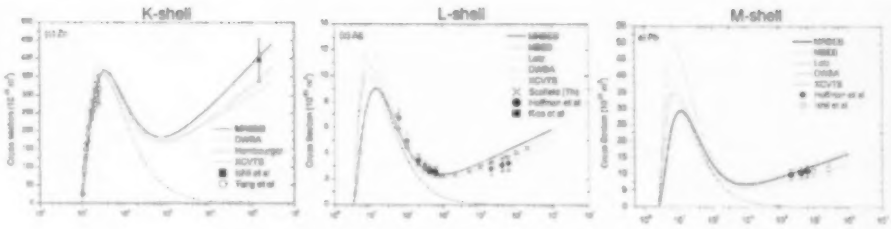
Regular Article

1–7

Modified binary encounter Bethe model for electron-impact ionization

M. Guerra, F. Parente, P. Indelicato, J.P. Santos

► We present a new method to calculate the ionization cross sections by electron impact. ► We calculatethe K-, L- and M-shell ionization cross sections by electron impact. ► Comparisons with all available experimental data prove the validity of the new model.

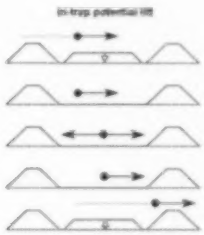


8–14

Static-mirror ion capture and time focusing for electrostatic ion-beam traps and multi-reflection time-of-flight mass analyzers by use of an in-trap potential lift

Robert N. Wolf, Gerrit Marx, Marco Rosenbusch, Lutz Schweikhard

► Ion injection and ejection can be accomplished without switching the mirror electrode potentials in electrostatic ion-beam traps andMR-ToF-MS. ► Ion-optical decoupling of the adjacent beam line ion optics from the storage device. ► Simplified optimization for high mass-resolving power.

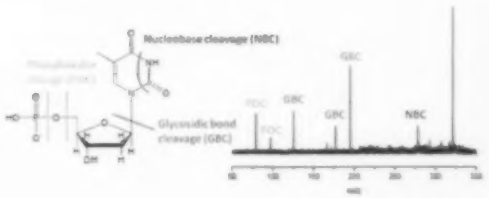


15–20

Metastable fragmentation of a thymidine-nucleotide and its components

Ilko Bald, Helga D. Flosadóttir, Benedikt Ómarsson, Oddur Ingólfsson

► Metastable decay of thymine nucleotides are characterized by N-glycosidic, phosphoester and nucle-obase ring cleavage. ► The initial deprotonation position determines the specific reaction pathway. ► Sugar cross-ring cleavage is only relevant for small DNA subunits. ► Formation of NCO− from thymineis due to deprotonation of N3. ► Presence of the phosphate group dominates fragmentation since itcarries the negative charge.



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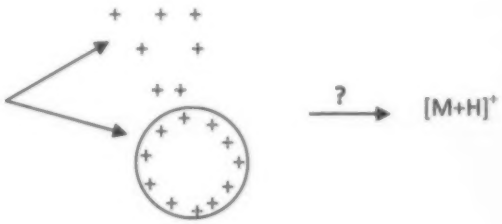
21–29

Mechanistic study on the ionization of trace gases by an electrospray plume

Pablo Martinez-Lozano Sinues, Ernesto Criado, Guillermo Vidal

► Electrospray ionization of vapors mechanism. ► Gas-phase analytes are not dissolved in the charged droplets to be ionized. ► Chemical ionization seems to be the leading mechanism.

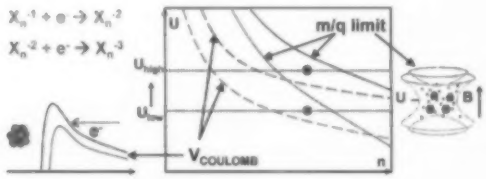


30–35

Lifting of the trapping potential during ion storage for multi-anion production in a Penning trap

Franklin Martinez, Steffi Bandelow, Christian Breitenfeldt, Gerrit Marx, Lutz Schweikhard, Frank Wienholtz, Falk Ziegler

► Multi-anionic clusters are produced in a Penning trap by electron attachment. ► For higher charge states, the Coulomb barrier interferes with trapping limitations. ► The multi-anion formation is performed stepwise with variation of the trapping potential. ► Metal-cluster penta-anions are produced for the first time.

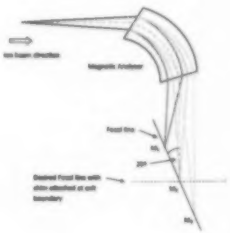


36–40

Rotation of focal plane of magnetic analyzer in an isotope ratio mass spectrometer using curved shims

Rajender K. Bhatia, Yogesh Kumar, K. Prathap Reddy, V.K. Yadav, E. Ravisankar, T.K. Saha, V. Nataraju, V.K. Handu

► This work includes the focal line slope determination on a thermal ionization mass spectrometer by theoretical calculations and computer simulations. ► Based on the theoretical and simulation results, iterative experiments have been conducted to find final parameters for the desired objective of rotation of focal line along normal to the principal beam axis. ► The final parameters were further confirmed by recording peak shapes on the actual setup.

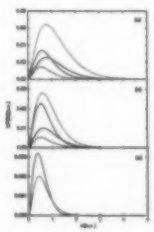


41–46

Electron loss accompanied by target ionization for He^+ and Li^{2+} on H and He in low- to intermediate-energy regime

Baowei Ding, Hongchao Li, Weijie Zhang

► We evaluate the electron loss cross sections for He^+, $Li2^+$ impacting on H and He. ► The calculated results are in general good agreement with the experiments. ► The range of the impact parameter for SL, SLSI and SLDI decrease in sequence. ► The present calculations can predict the peak position correctly. ► The peak position depends on the effective charges and the binding energy.

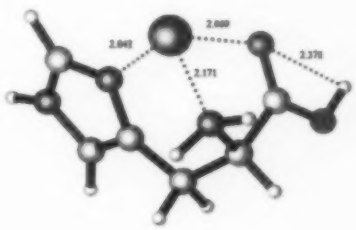


47–57

A theoretical elucidation of coordination properties of histidine and lysine to Mn^{2+}

M. Hassan Khodabandeh, Hamid Reisi, Karim Zare, Mansour Zahedi

► Interaction between histidine and lysine with Mn^{2+} in the gas phase by quantum chemical calculations. ► Three types of complexation mode have been considered: (i) three dentate chelation of neutral amino acids; (ii) two dentate chelation of neutral amino acids; (iii) chelationof amino acids to metal ion in zwitterionic forms. ► The most stable structure resulted from interaction of neutral amino acids with metalcation via two amino groups and carbonyl oxygen.

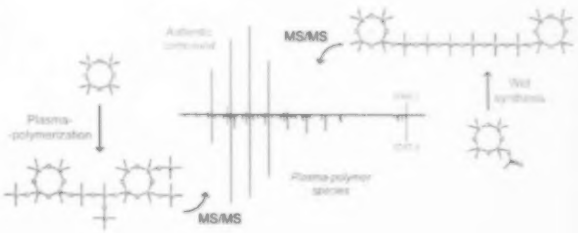


58–67

Electrospray tandem mass spectrometry combined with authentic compound synthesis for structural characterization of an octamethylcyclotetrasiloxane plasma polymer

Thierry Fouquet, Julien Petersen, Joao A.S. Bomfim, Jérôme Bour, Fabio Ziarelli, David Ruch, Laurence Charles

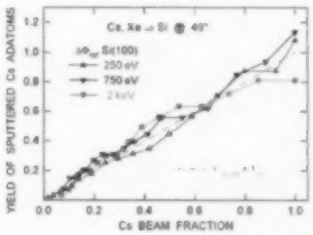
► CID was used to investigate the structure of a plasma polymer. ► Authentic compounds were synthesized to assign product ions in MS/MS. ► This plasma polymer was found to be a branched cyclolinear polysiloxane.



Short Communications

68–72

Mechanisms responsible for inducing and balancing the presence of Cs adatoms in dynamic Cs based SIMS

Klaus Wittmaack

► The work function changes produced by Cs implantation are revisited. ► It is shown that implanted Cs atoms are rapidly transported tothe sample surface. ► Prior to being sputtered, implanted atoms are transiently converted to adatoms. ► The rates of Cs implantation and reemission of adatoms are in balance within ± 20%.